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Applied Mechanics and Materials Vols. 446-447 (2014) pp 790-795
Online available since 2013/Nov/08 at www.scientific.net
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doi:10.4028/www.scientific.net/AMM.446-447.790

Solid Oxide Fuel Cell and Steam Reformer System Steady State Modeling

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Keywords: Ethanol, Solid oxide fuel cell, Steady state modeling, Steam reformer.

Abstract. A solid oxide fuel cell (SOFC) is widely recognized to be an attractive energy conversion device owing to its fuel flexibility and high efficiency. Hydrogen-rich stream produced by fuel processor, especially steam reforming process, is used as fuel carrier converting to generate electrical energy. This paper presents a steady state modeling of SOFC system with an integrated steam reformer fueled by ethanol. The main objective of this study is to analyze the steady state characteristics of this system. The basic operating principle of SOFC is briefly introduced and the steam reformer converting ethanol as the fuel source into hydrogen-rich gas is also discussed. Based on thermodynamic analysis, the equilibrium compositions of produced gas fed into SOFC can be predicted by using the method of Gibbs free energy minimization. The effects of main operating parameters of steam reformer including the temperature and water-to-ethanol molar ratio on the SOFC power generation are investigated. In the SOFC operation, an increase of SOFC temperature causes a decrease of cell voltage and an increase of excess air entering a fuel cell to maintain the adiabatic temperature of SOFC stack. The steady state conditions for the SOFC and ethanol steam reformer systems are summarized in this paper as well.

Introduction

As the world confronts many serious problems about global warming and atmospheric pollution from direct fossil fuel combustion and continuously increasing fuel prices, hydrogen is repeatedly considered to be an alternative fuel for fuel cells because of its clean energy and environmental reasons. Among different types of fuel cells, it is known that a solid oxide fuel cell (SOFC) can offer the widest potential range of applications and high system efficiency [1]. The SOFC is remarkably interesting because of its high operating temperature range between 1073 and 1273 K such a high temperature allows the use of non-noble catalysts which can not be poisoned by carbon monoxide that makes it highly fuel-flexible. Therefore, hydrogen-rich gas produced by fuel processor can be directly fed into an anode side of SOFC for generating electricity. From an environmental point of view, the use of ethanol is favored because ethanol could be considered as a renewable raw material easily produced from biomass fermentation. Ethanol is very attractive as it has a relatively high hydrogen content, and it is non-toxic, easy to store and transport. Ethanol has a considerable benefit of being nearly carbon dioxide neutral since carbon dioxide produced in the process is consumed for biomass growth, thus offering a nearly closed carbon loop [2]. Therefore, in this present work ethanol is chosen as the fuel for hydrogen production.

Three main fuel processors for hydrogen production are steam reforming, catalytic partial oxidation, and oxidative steam reforming, also called autothermal reforming. Most traditional hydrogen production is a kind of catalytic reforming reaction on a catalytic bed reactor. The endothermic reaction of steam reforming is widely applied for hydrogen production because it can offer the highest concentration of hydrogen content from hydrocarbon fuels [3]. Liso et al. [4] compared two different types of pre-reforming systems, namely, steam reforming and partial oxidation for SOFC fueled by natural gas (or methane), and the results showed that methane steam reforming produces a higher electrical efficiency compared to partial oxidation process. Das et al. [5]

performed the steady state and transient analysis of a steam reformer based SOFC system to analyze the steady state and transient behaviors of two critical performance variables, namely, fuel utilization and steam-to-carbon balance. Additionally, most of the previous work on the SOFC system integrated with steam reformer has focused on the use of methane as a fuel for hydrogen production [4-7]. Srisiriwat et al. [8] presented SOFC integrated with different fuel processors fueled by ethanol that the efficiency of hydrogen production and SOFC power generation with various technologies of hydrogen production was compared, but there have been no reports on the effect of water amount for steam reforming reaction and of reforming temperature on the steady state operating condition of SOFC which is very useful for process design and control.

As mentioned above, a steady state modeling of SOFC system integrated with a steam reformer fueled by ethanol has been performed. The effects of reforming temperature and water-to-ethanol (H_2O:EtOH) molar ratio on the hydrogen yield and SOFC operating conditions are investigated. The minimum Gibbs free energy method is used to determine the equilibrium compositions of hydrogen production. The steady state conditions of the operation of SOFC and steam reformer systems are also reported in this paper.

SOFC and steam reformer system modeling

The system of solid oxide fuel cell (SOFC) integrated with steam reformer fueled by ethanol is illustrated in Fig. 1. The system consists of pumping devices, including liquid pumps and air compressor, heat exchangers, steam reformer and SOFC stack. The ethanol fuel is pumped to mix with water and preheated before entering a steam reformer at which the high energy for the endothermic reaction is required. The ideal pathway of ethanol reforming for the maximum hydrogen production is the complete conversion to hydrogen and carbon dioxide as follows:

$$C_2H_5OH + 3H_2O \qquad 6H_2 + 2CO_2, \qquad \Delta H^{o}_{298} = 173.5\ kJ/mol \tag{1}$$

However, in fact, the stoichiometric coefficient of hydrogen can not reach 6 since in the steam reforming conditions other ethanol reactions can take place such as decomposition, dehydrogenation, etc. The hydrogen-rich gas is produced in the reformer and then fed into the anode side of SOFC. Air is compressed and preheated before entering the cathode side. Inside the fuel cell, the SOFC reactions that take place at anode and cathode to generate both of the electricity and heat can be described as:

$$\begin{aligned} &\text{Anode:} && H_2 + O^{2-} \quad H_2O + 2e^- \\ &\text{Cathode:} && \tfrac{1}{2}O_2 + 2e^- \quad O^{2-} \\ &\text{Overall:} && H_2 + \tfrac{1}{2}O_2 \quad H_2O \end{aligned} \tag{2}$$

Component models capable of correctly predicting the performance of SOFC and steam reformer were implemented in steady state condition. The fluid properties at inlet and outlet remain constant [4]. The mass balance for a general steady state system can be written as

$$\sum_{in} \dot{m} = \sum_{out} \dot{m} \tag{3}$$

The total energy content remains constant, and thus the change in the total energy of the control volume is zero [4].

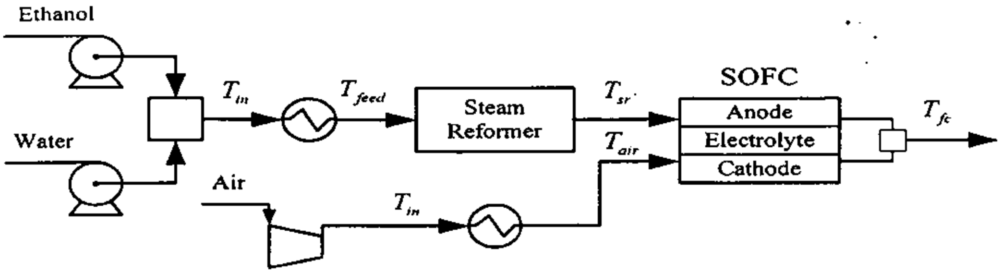

Fig. 1. SOFC and ethanol steam reformer system.

Model general assumption. To assist low computational time and numerical stability, the system has been modeled under various simplifying assumptions described as:

- Each system component is considered as control volume.
- Ethanol is used as fuel source for hydrogen production by steam reformer that the minimum Gibbs free energy is applied to predict the equilibrium compositions.
- Carbon formation in the system is not modeled, since it is assumed to avoid by using the high amount of water content mixed with ethanol.
- Air is approximated to consist of 21% oxygen and 79% Nitrogen.
- Pressure losses owing to piping are neglected.
- All the physical properties are assumed to be uniform over the SOFC, resulting in a lumped model.
- All the gases are assumed to be ideal.
- For the energy balances, the changes of pressure within the SOFC are neglected.
- The temperature of fluids leaving the stack is equal to the stack temperature.
- An adiabatic operation of the fuel cell is assumed.
- The system is evaluated at steady state, negligible transient effects.
- The SOFC system is assumed as being thermodynamic lumped model.

Fuel cell modeling. As the operating temperature of SOFC is known, the total inlet and outlet flow of air can be determined by the conservation of equations. The air inlet stream is contained two functions for the SOFC system; the first function of air fed to the cathode side of SOFC is for electrochemical reactions in the SOFC and the second purpose of air fed is for the cooling system to maintain the adiabatic SOFC process. In order to control the SOFC temperature, an energy balance is set up and the air molar flow is considered to be a variable. The energy balance of the SOFC stack is defined as follow:

$$\Sigma \dot{m}_{i,in} h_i (T_{sr} - T_{ref}) + \dot{m}_{air} h_{air} (T_{air} - T_{ref}) = \Sigma \dot{m}_{i,out} h_i (T_{fc} - T_{ref}) + \dot{n}^r_{H_2} \Delta H^\circ_r + V_s I \qquad (4)$$

where $\dot{m}_i$ is the mass flowrate of species i, h the enthalpy, T the temperature as referred in Fig. 1, T_{ref} the reference temperature (298 K), $\dot{n}^r_{H_2}$ the molar flowrate of reacted hydrogen, ΔH°_r the heat of reaction at STP, V_s the cell voltage and I is the current.

The fuel utilization factor (U_f) is the main parameter for calculating the molar flowrate of reacted hydrogen as follows:

$$U_f = \frac{\dot{n}^r_{H_2}}{\dot{n}_{H_2,in} + \dot{n}_{CO,in} + 4\dot{n}_{CH_4,in}} \qquad (5)$$

where $\dot{n}_{i,in}$ refers to the anode's fuel species input. For achieving a desired U_f the amount of reacted oxygen passing through the cathode is specified as $\dot{n}^r_{O_2} = 0.5\dot{n}^r_{H_2}$ [9].

The operation cell voltage (V_s) is given by

$$V_s = V_{OCV} - V_{loss} \tag{6}$$

where the open circuit voltage of the cell, V_{OCV} is given by the Nernst equation [10],

$$V_{OCV} = E_o(T_{fc}) + \frac{RT_{fc}}{2F}\ln\left(\frac{p_{H_2}p_{O_2}^{0.5}}{p_{H_2O}}\right) \tag{7}$$

and

$$E_o(T_{fc}) = 1.185 - 0.2302x10^{-3}(T_{fc} - T_{ref}) \tag{8}$$

where $E_o(T_{fc})$ is the standard cell potential and p_{H_2}, p_{O_2} and p_{H_2O} are the partial pressures of hydrogen, oxygen and water, respectively. The voltage loss resulting in the lower actual voltage delivered by the fuel cell is less than the open circuit voltage due to activation, ohmic and concentration polarization as described in ref. [10].

The total current can be calculated by following equation

$$I = 2F\dot{n}_{H_2}^{r} \tag{9}$$

where F is the Faraday's constant (96,484 C/mol).

The cell power output is

$$P = V_s I \tag{10}$$

Results and Discussion

The effects of steam reforming temperature on the product distributions were obtained by using the method of minimization of Gibbs free energy as shown in Fig. 2. The reaction temperature had a significant effect on the gas compositions in the product stream. An increase of the temperature considerably increased the hydrogen gas composition and rapidly decreased the methane content. The maximum hydrogen composition was obtained at the temperature of 973 K and above this temperature, the hydrogen and carbon dioxide decreased when the amount of water and carbon monoxide increased because of the reverse water gas shift reaction. The reforming temperature of 973 K was presented as the optimum operating temperature for steam reformer.

Table 1 shows the effect of H_2O:EtOH ratio on the SOFC operation at reforming temperature of 973 K and SOFC temperature of 1200K. An increase of water amount in the steam reformer system increased the efficiency of hydrogen production causing an increase of SOFC power generation. To compare the efficiency of hydrogen production from steam reformer, the fuel utilization is calculated by Eq. 5 that reacted hydrogen is converted to be electrical energy. Therefore, the maximum fuel utilization increased with increasing the hydrogen yield. The higher fuel utilization, the higher power generation that caused the higher of exothermic energy of SOFC heat load. The excess air was fed into SOFC in order to sustain SOFC adiabatic operation. The results showed that the amount of excess air increased as the exothermic energy of SOFC increased.

The effect of temperature in steam reformer on SOFC conditions at H_2O:EtOH ratio of 10 and SOFC temperature of 1200 K is shown in Table 2. The reforming temperature had a notably effect on the hydrogen yield as well as the maximum fuel utilization and SOFC power generation. The optimum hydrogen production was obtained at steam reformer temperature of 973 K considered as the best condition for the SOFC integrated with steam reformer system. The maximum SOFC power generation was 663 kW with the fuel utilization of 0.9 and excess air of 74.9 mol/s.

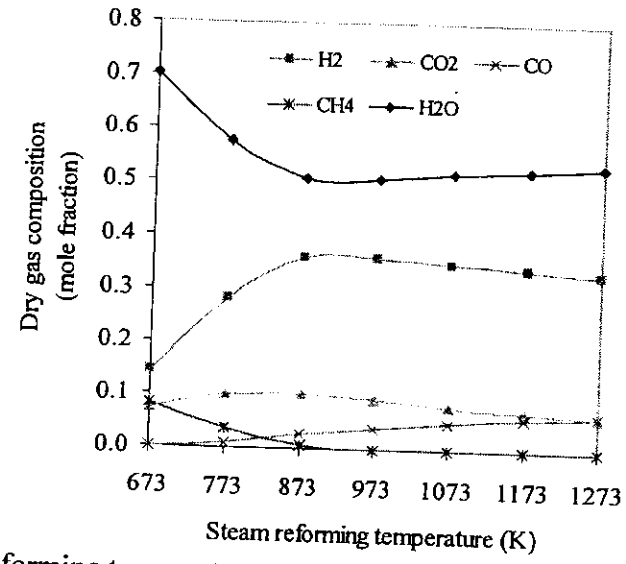

Fig. 2. Effect of steam reforming temperature on equilibrium compositions at H_2O:EtOH ratio = 10.

Table 1 Effect of H_2O:EtOH ratio on SOFC parameters at temperature of steam reformer = 973 K and SOFC temperature = 1200K

H_2O:EtOH ratio	**H_2 yield**	**Maximum fuel utilization [U_f]**	**SOFC power generation [kW]**	**SOFC heat load [kW]**	**Excess air [mol/s]**
2	3.87	0.64	554	-834	59.5
3	4.38	0.73	604	-892	63.7
4	4.69	0.78	631	-931	66.5
6	5.05	0.84	653	-982	70.1
8	5.25	0.87	662	-1018	72.7
10	5.38	0.90	664	-1049	74.9

Table 2 Effect of temperature of steam reformer on SOFC parameters at H_2O:EtOH ratio = 10 and SOFC temperature = 1200 K

Steam reformer temperature [K]	**H_2 yield**	**Maximum fuel utilization [U_f]**	**SOFC power generation [kW]**	**SOFC heat load [kW]**	**Excess air [mol/s]**
673	1.84	0.31	226	-845	60.4
773	3.92	0.65	483	-1006	71.8
873	5.32	0.89	657	-1096	78.3
973	5.38	0.90	663	-1049	74.9
1073	5.23	0.87	646	-979	69.9

Fig. 3 illustrates the effect of SOFC temperature on the cell voltage and amount of excess air. It was observed that an increase of SOFC temperature decreased the cell voltage but increased the excess air required to maintain the adiabatic temperature of SOFC.

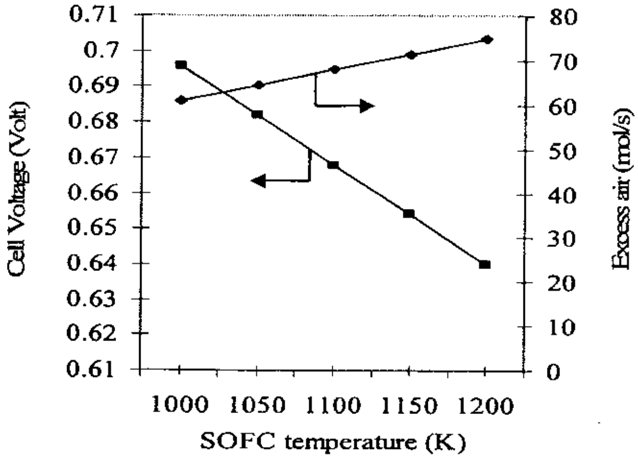

Fig. 3. Effect of SOFC temperature on cell voltage and excess air.

Conclusion

As hydrogen is considered as the alternative energy for fuel cell, in this study, the ethanol steam reforming is applied for fuel processor. A steady state modeling of solid oxide fuel cell (SOFC) integrated with steam reformer systems has been investigated. The effects of steam reformer conditions on the efficiency of hydrogen production and SOFC power generation were presented that an increase of water amount and temperature in steam reformer increased the hydrogen yield resulting in the higher SOFC power generation. The SOFC temperature had an effect on cell voltage and excess air. In the SOFC operation, an increase of SOFC temperature caused a decrease of cell voltage and an increase of excess air entering a fuel cell to maintain the adiabatic SOFC process.

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Publisher: Trans Tech Publications. **Publication type:** Book Series. **ISSN:** 16609336, 16627482

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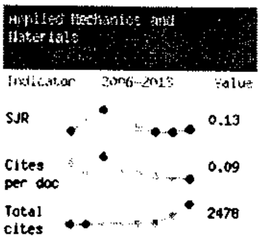

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